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In-situ STM analysis and photoluminescence of C-induced Ge dots

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Abstract. Molecular beam epitaxy has been utilised to grow small C induced Ge islands in silicon. Using in-situ STM analysis, it is shown that the amount of C deposited on the Si(100) surface prior to Ge growth permits the control of lateral size and height of Ge quantum dots. The Ge grows in a Volmer-Weber growth mode in areas between the C-rich patches on the Si surface. Thus laterally smaller but higher dots are found with increasing C coverage. Accordingly, intense photoluminescence (PL) with a stronger confinement shift in dependence on the Ge coverage is observed for samples prepared with large C concentrations. The impact of the Si spacer layer width on the dot size has been studied by TEM and compared to PL data.

Introduction

The search for paths to integrate optoelectronic devices in the mature Si technology has lead to various techniques for the fabrication of nanostructures in Si. The one taken up in this study is the formation of small Ge dots on Si(100) surfaces covered with sub-monolayers of C [1]. It has been shown that using this technique the lateral island size can be reduced below 20 nm at growth temperatures in the range of 500°C. These growth temperatures provide excellent crystalline quality and consequently pronounced photoluminescence (PL) was observed for these C-induced Ge quantum dots [2]. However, even smaller and more compact islands are required to further tailor the PL intensity. Previously study we showed using in-situ STM analysis that the C forms patches exhibiting a c(4×4) reconstruction, whereas the areas between these C rich patches remain free of C and exhibit buckled Si dimer rows [3]. Here we explore the Ge nucleation on the C alloyed Si surface. It is found that C can be used to limit the area available for the nucleation of the Ge dots. Using the amount of deposited C and Ge as growth parameters, samples containing multiple layers of C-induced Ge dots have been fabricated by MBE at 460°C. Additionally the Si spacer layer has been varied to study its impact on the structural and optical properties of the dots. Furthermore, transmission electron microscopy (TEM) and PL has been used to investigate the dots embedded in Si. A sensible correlation of the gathered features yields insights into the peculiarities of C-induced Ge dots, with respect to the carrier confinement.

Results and discussion

Figure 1(a) shows the evolution of 3-dimensional (3D) islands on the C-alloyed Si surface. The STM image is taken after the deposition of 0.1 monolayer (ML) of C and 1 ML of Ge at 550°C and 350°C, respectively. The Ge does not cover the whole surface but instead grows in 3D piles. In areas between the islands the unperturbed c(4×4) reconstruction is visible [3]. The density of Ge islands amounts to 8×10^{11} cm^{-2}, the diameter to 4–5 nm and the height up to 6 ML. The line scan in Fig. 1(a) is taken at the position indicated by the white line in the STM image. The islands show an irregular shape of the basis, in contrast to lower Ge coverages (0.1–0.5 ML), where rectangular island shapes are most often observed. No

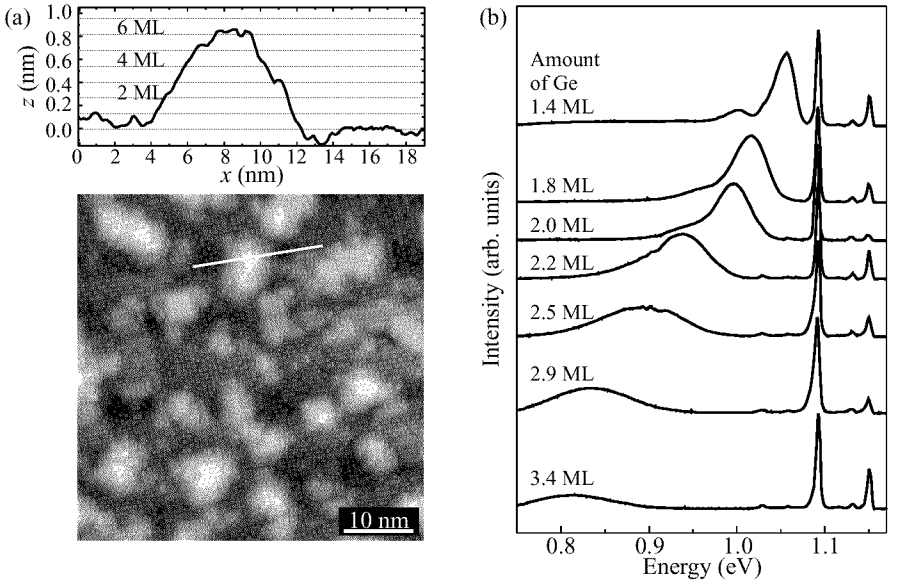

Fig. 1. (a) STM surface images and line scan of C-induced Ge dots (0.2 ML C, 1 ML Ge). (b) 2.8 K PL spectra of C-induced Ge islands fabricated with various amounts of Ge ML.

distinct facet reconstruction can be seen, because the side walls are irregular. Nevertheless a certain affinity to side facet formation either in ⟨100⟩ or ⟨110⟩ directions is visible. Due to the freedom to expand in 3 dimensions, the islands are presumably relaxed towards their apex. The height to base ratio is approximately 1/10, which is similar to relaxed pure Ge hut clusters [4].

It is important to notice that no Ge wetting layer is formed. We assume that no Ge is incorporated into the C rich c(4×4) reconstructed areas, since this would almost certainly alter the appearance of these regions in STM. Most likely the C patches are highly strained due to the big lattice mismatch between Si and C, thus the lattice constant in the C rich region is smaller than that of Si. Ge expands the Si lattice and is therefore easier accommodated on the Si surface free of C.

At higher deposition temperatures for the Ge, up to 550°C the islands tend to become flatter. But the general feature, that no Ge wetting layer is formed and that the island start to nucleate in regions free of C, persists. STM images taken for Ge islands formed by 2 ML indicate that finally the c(4×4) reconstructed areas vanish [5]. Apparently the C rich areas are overgrown by Ge, however, it is unknown how the C is incorporated into the crystal at this stage. The C deposition in Fig. 1(a) is only 0.1 ML, at higher C coverages, up to 0.3 ML, the area available for Ge nucleation becomes even smaller leading to a smaller lateral size and to an increase in the height to base ratio.

Figure 1(b) shows the dependence of PL spectra of C-induced Ge dots (0.2 ML C) on the amount of Ge deposited. The samples, grown at 460°C, contained 10 layers of dots separated by 8 nm wide Si barrier layers. All samples were annealed at 650°C for 4 min subsequent to growth, leading to an intensity increase by a factor of 2 to 4, whereas the change in the energetic peak positions is minor. The increase from 1.4 to 3.4 ML Ge leads to an energy shift of approximately 250 meV. The peak intensity drops significantly for Ge depositions exceeding 2.5 ML, indicating a weaker 0-dimensional localisation in

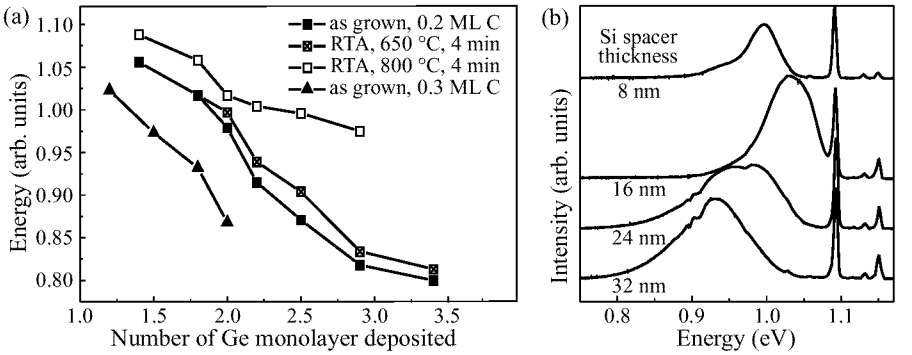

Fig. 2. (a) Confinement shift of C-induced Ge dots, for as deposited dots ($T = 460°C$) and after RTA processing for 4 min at 650 and 800°C in a 4% H_2/N_2 gas mixture. (b) Dependence of the Si spacer thickness.

larger dots.

In Fig. 2(a) the energetic position of the peak maximum of the dot related PL is plotted in dependence on the number of Ge monolayers deposited on top of the 0.2 ML of C. A strong confinement shift is observed in the region between 3 and 1.8 ML, for smaller dots the shift saturates. Since the dots have the shape of platelets, and their dimensions in the xy plane are much larger than their heights, the height of the islands determines predominantly the confinement shift.

The saturation in the confinement shift for islands formed by less than 1.8 ML might be attributed to the heavy hole state in the Ge dot area approaching the Si band edge. Also annealing at 800°C has only little impact on the peak position for these very small dots, which fits to the latter conclusions. C on lattice sites does not diffuse in the temperature range of 800°C. Annealing leads to an intermixing of Si and Ge, thus to bigger dots with a lower Ge content, which explains the strong shift towards higher PL energies collected from the large dots. For small dots, where the subband level of the holes is shifted close to the band edge by the confinement, the annealing has only a minor effect. The difference in the peak energy between the dot PL for very small dots and the Si NP peak at 1150 meV is only in the range of 50–60 meV, which might be the confinement energy of the electrons in the C rich Si. The highest peak as well as integrated intensity is found for dots deposited with 1.8–2.2 ML of Ge. For smaller dots the confinement shift saturates; the localisation of the wavefunction is weak when the quantum state in the well approaches the band edge of Si, thus the matrix element decreases.

As found by TEM analysis, also the shape of the Ge dots is affected by the amount of C deposited. They grow in height at the expense of their diameter at higher C coverages. The C-covered area increases for higher amounts of C deposited, whereas the local density of C within the C covered areas is constant, as indicated by the c(4×4) reconstruction detected by STM. The PL lines shift significantly to lower energies with increasing C contents. The peak positions of a series of samples grown with 0.3 ML of C are also indicated in Fig. 2(a) (closed triangles). They are significantly shifted to lower energies for the same amount of Ge deposited, when compared to those of dots induced by 0.2 ML C. This is attributed to the increase in dot height.

Figure 2(b) shows four PL spectra of Ge dots fabricated by depositing 2 ML Ge on top of 0.2 ML C, each comprising 10 layers separated by 8, 16, 24 and 32 nm Si spacer

layers. Surprisingly, the PL shifts by 35 meV to higher energies, if the spacer thickness is increased from 8 to 16 nm. At the same time the intensity increases. This can be understood by assuming an overlap of the wavefunctions confined in adjacent dot layers, leading to a system of weakly coupled dots. A further increase of the Si spacer thickness leads to a red shift and a broadening of the lines.

The latter effect is difficult to explain. To gather more detailed insights into these samples, they have been carefully analysed by TEM. Surprisingly, the dot size is smaller for the 16 nm wide Si buffer layers as for layers grown with 24 and 32 nm wide barriers.

Conclusions

In conclusion, clear indications of a zero dimensional confinement were detected. It increases, when the C coverage of the surface is increased, thus the C free area shrinks, leading to a more compact shape of the Ge islands. They grow in height and reduce their lateral dimensions. The results indicate that the electrons are confined in the C-rich areas between the dots and that the holes are confined in the Ge dots. The recombination is a spatial indirect process. This makes the design for optimised PL efficiency quite complex. On the one hand side a strong localisation of the wavefunction in local space is desired to overcome the indirect bandgap in k-space. On the other hand side an overlap of the electron and hole wavefunctions in local space is required to increase the possibility of the spatial indirect recombination.

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